Characterization and Modeling of Interfaces and Interphases in Polymeric Systems

F.R. Phelan Jr.

Polymers Division, NIST

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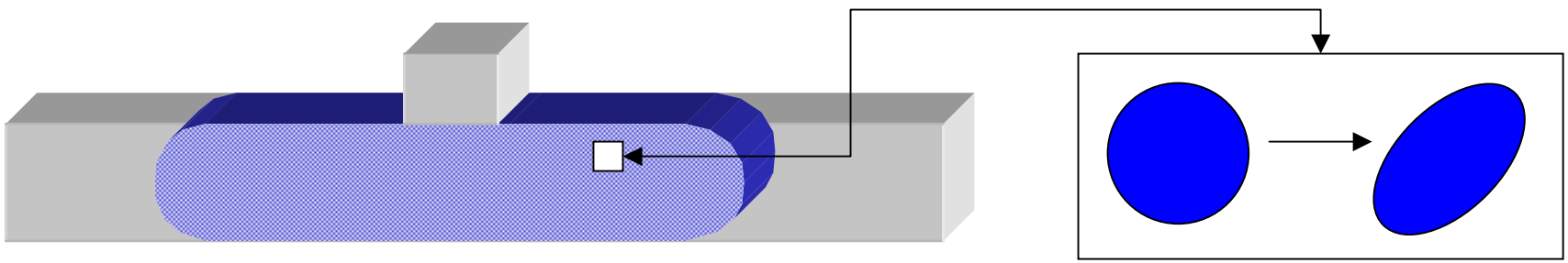
Consortium Update

Interface and Interphase Morphology Project

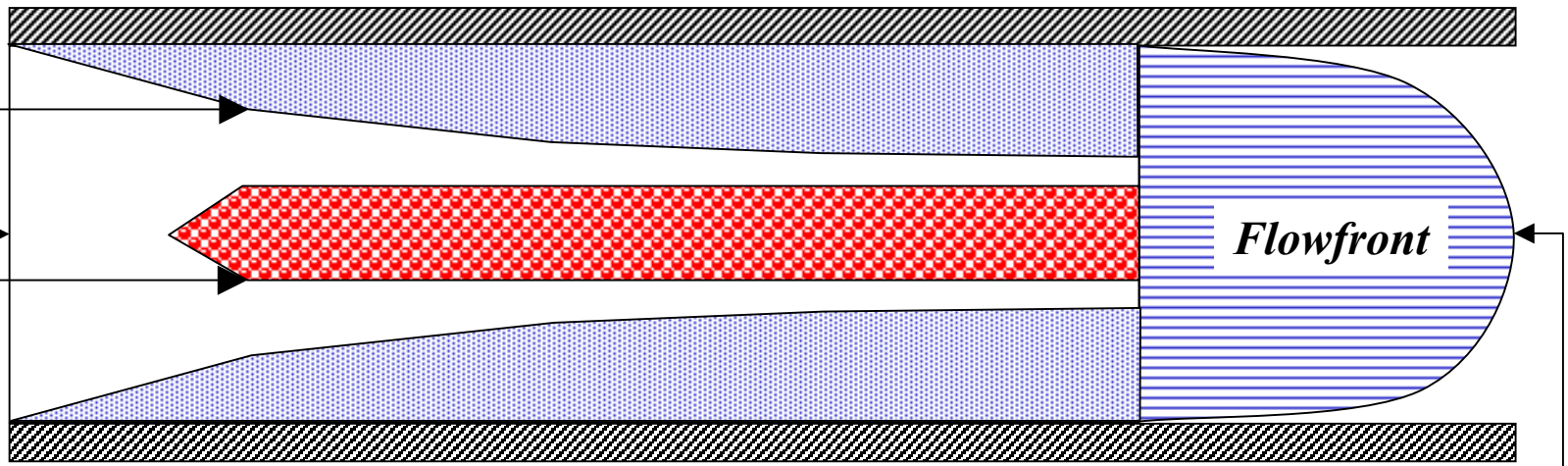
- **Injection molding of two-phase systems**
  - » **Predict injection molding filling**
  - » **Predict drop size distribution/morphology**



Polymer Blend Injection Molding

Inflow -- Well mixed extrudate

Wall Region -- High Shear, Stretching and Breakup, Small Drops

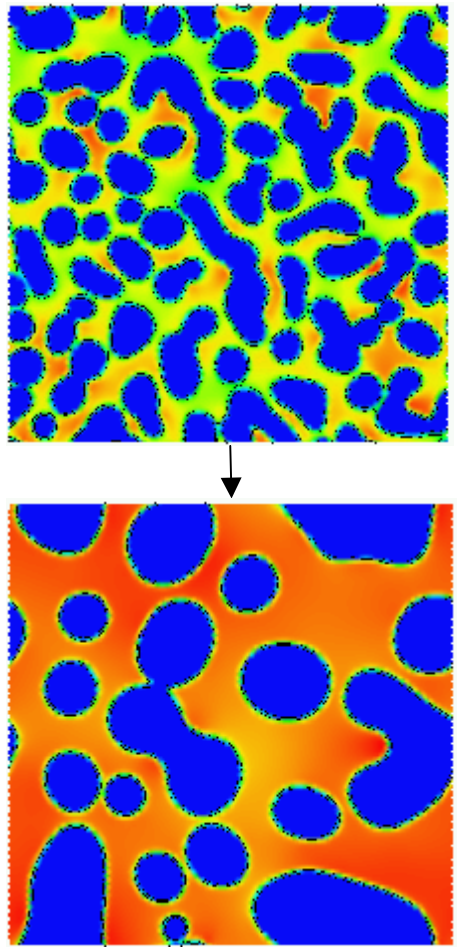


Center -- Low Shear, Coarsening, Larger Drops

Flowfront -- Extensional Flow, "Front to wall flow"

Direct Multiphase Simulation

- **"Diffuse Interface" Models**
  - » **e.g., Ginzburg-Landau, Lattice Boltzmann**
- **Difficulty: mismatched size scales**
  - » **Drop scale, microns**
  - » **Mold scale, cm to m**
- **Impractical for injection molding**



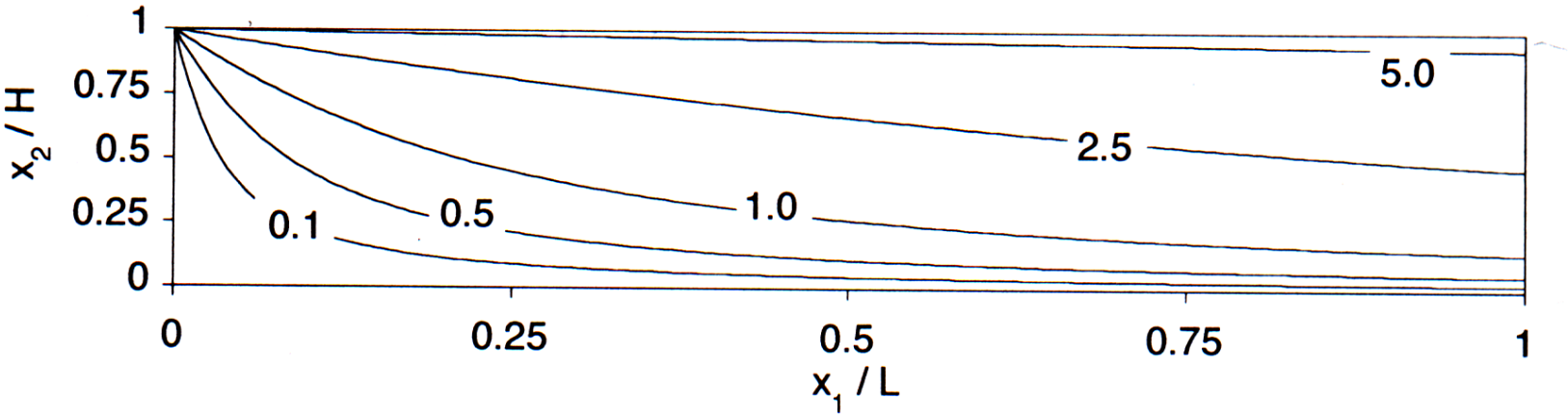
Ripening in spinodal decomposition; simulation by M.A.A. Spaid, F. Phelan, via Lattice Boltzmann

Multiphase Flow Models

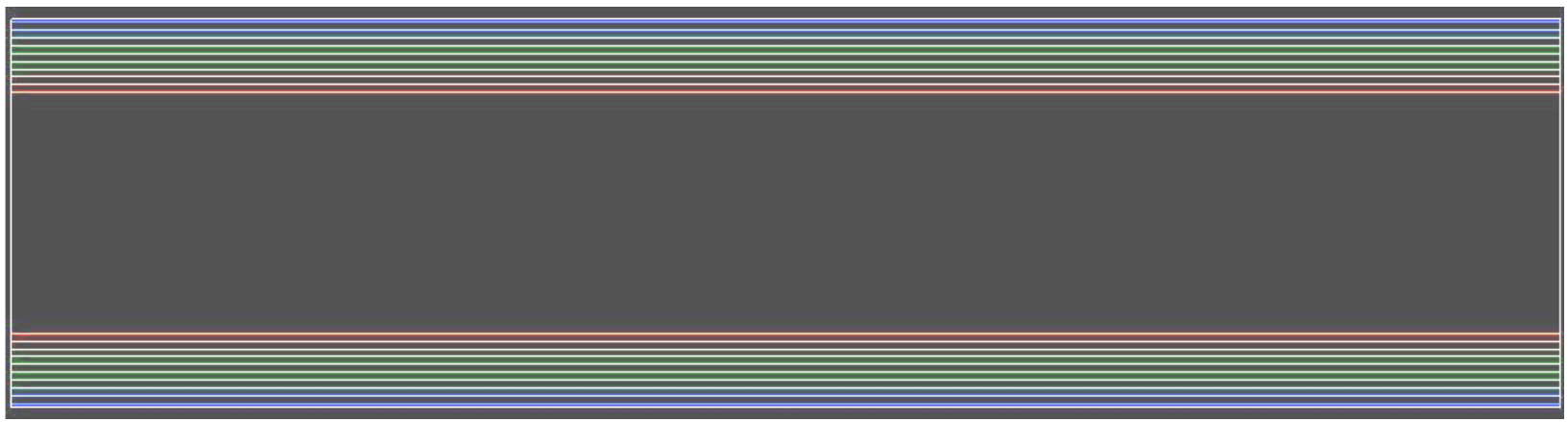
- **Averaging Methods**
  - » **Phase averaged properties**
  - » **Predict microstructure from micro- or phase averaged model**
- **Models**
  - » **Data Based Models**
    - ***Phase averaged properties***
    - ***Little or No Dynamics***
  - » **Hierarchical Modeling**
    - ***Combination of multiple simulation techniques at several length scales***
  - » **Tensor Methods**
    - ***Phase averaged properties***
    - ***Extensions to complex flow dynamics***

Comparison with Tensor Model

Tucker and Wetzel, Area Tensor, 1998

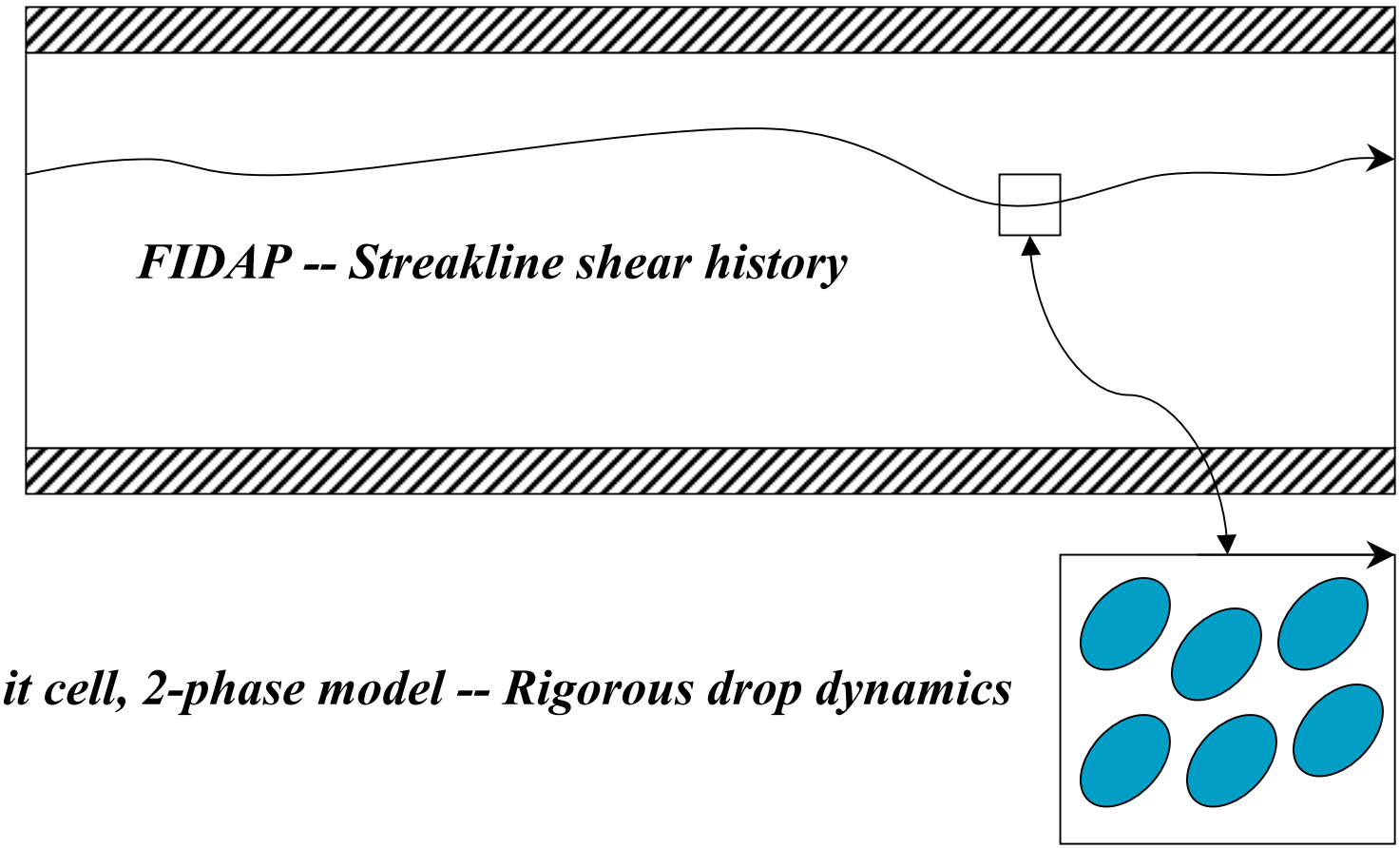


Present Work



Drop size, PB/PI:55/45

Hierarchical Multiphase Modeling

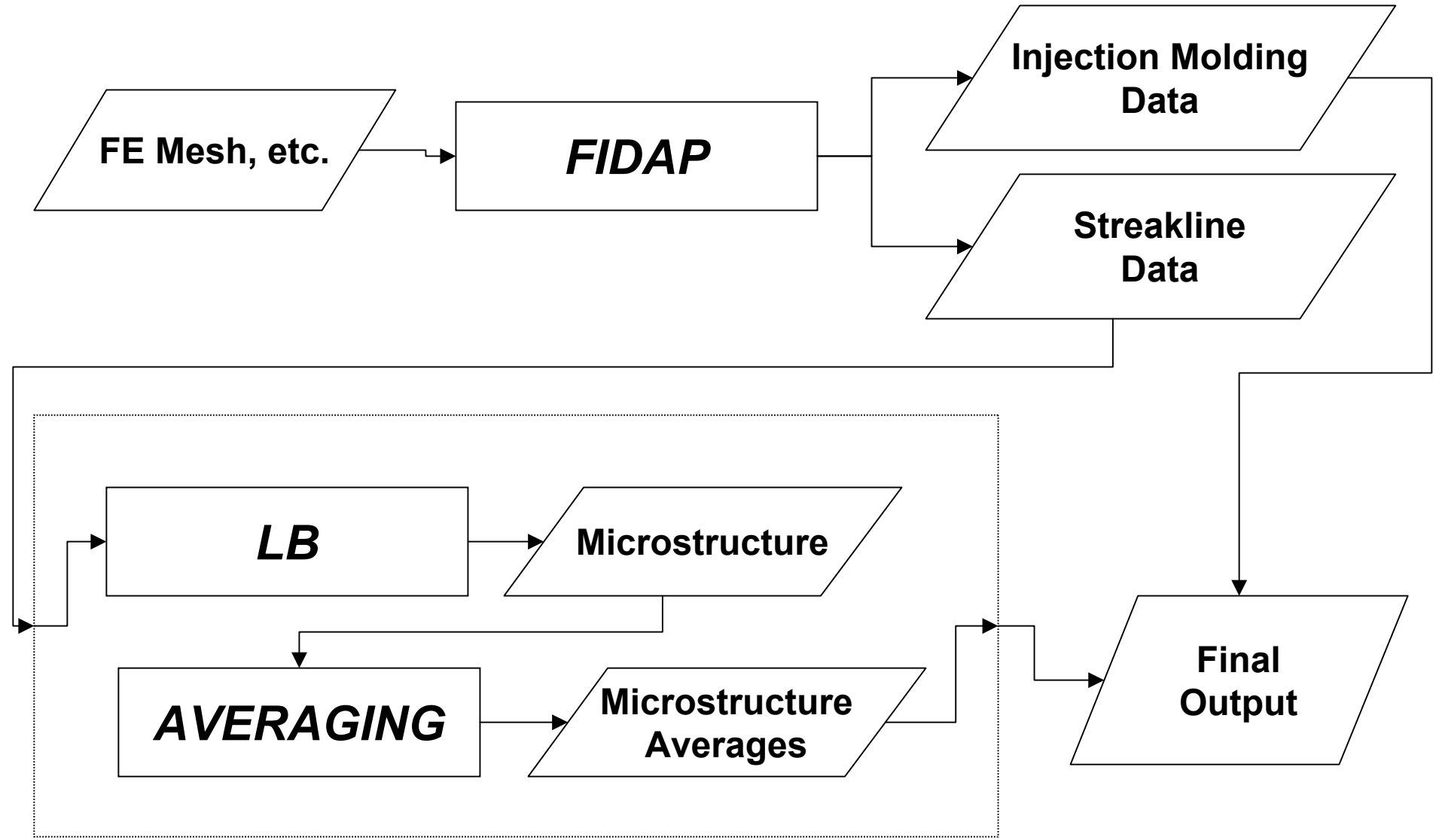


Unit cell, 2-phase model -- Rigorous drop dynamics

Hierarchical Multiphase Modeling

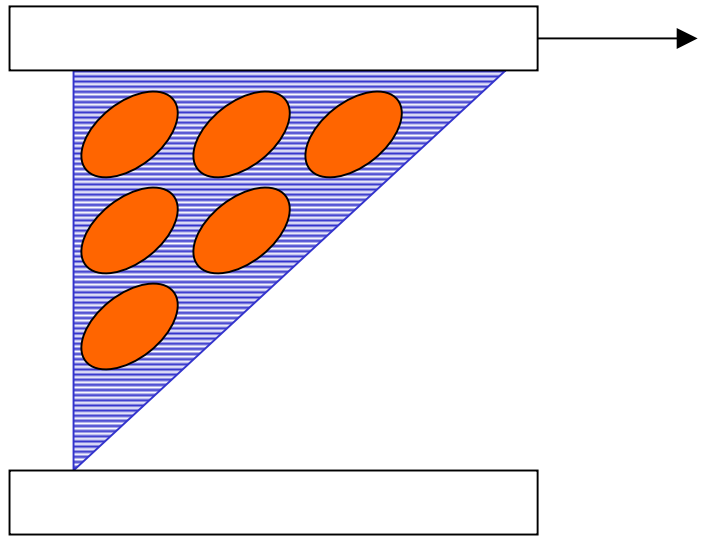
- **Goals**
  - » Average size and orientation
  - » Phase separating systems
  - » Dynamics of breakup
- **FIDAP Adaptation**
  - » Add user defined subroutine for blend viscosity
  - » Compute flow field and “streaklines”
- **Direct two-phase calculations on streaklines**
  - » Detailed microstructure prediction
  - » Compute averages

Injection Molding Algorithm



Multiphase Flow Modeling (Microflow)

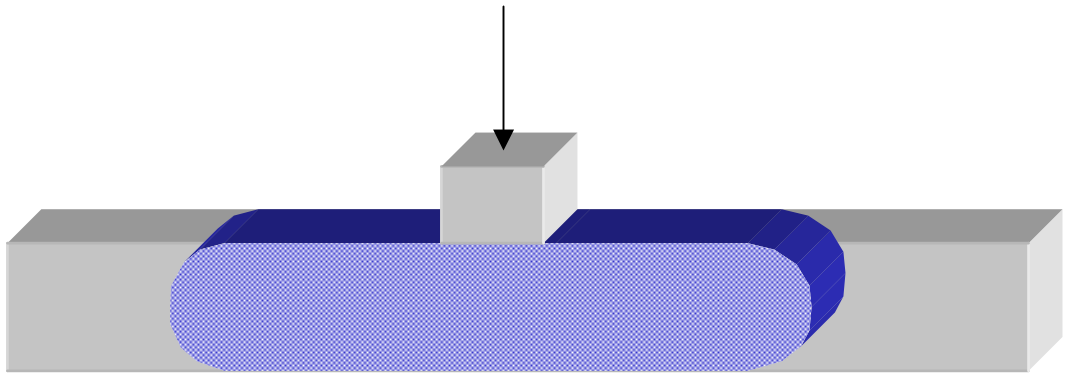
- **Methods**
  - » **Lattice Boltzmann Methods, 3-D (Martys, Phelan)**
  - » **Multi-component Navier-Stokes model (2-D)**
- **Boundary conditions on unit cell set from shear history along streaklines**
- **Initial condition set by feed condition at entrance to injection molding die**



Unit Cell

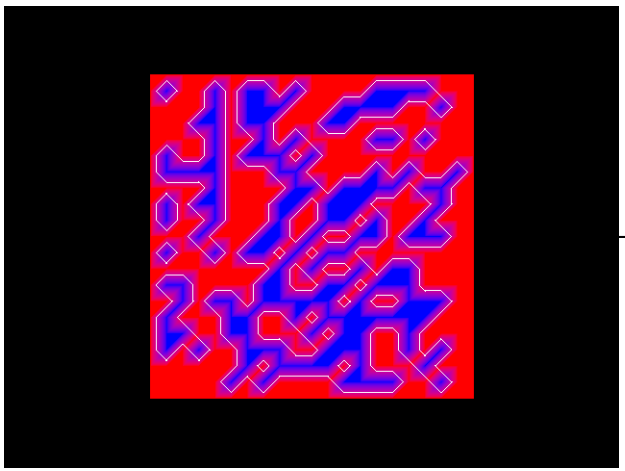
Example: Injection Molding of Phase Separating System

Feed From Extruder: Phase Separating

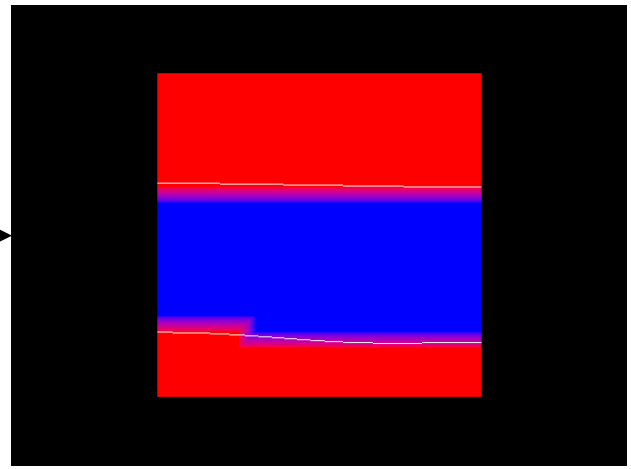


Multiphase Calculation: 2-D Shear Flow

Initial Condition: Random, 40% Blue



K_{ch}=0.01, t=38.5



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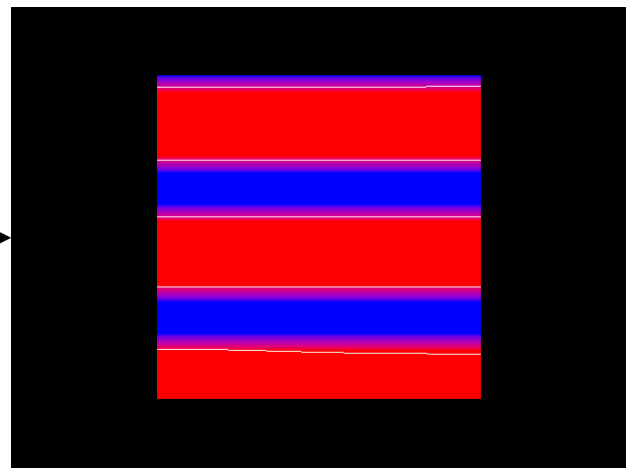
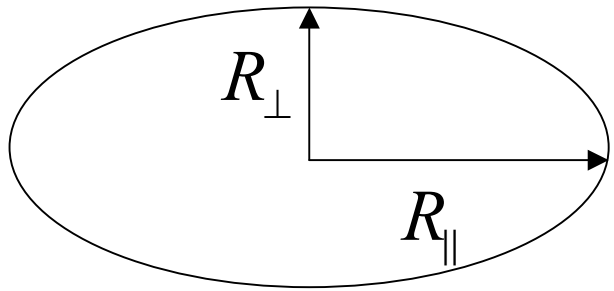


Growth Laws

$$R_{\parallel} = R_{\parallel 0}\left(\dot{\gamma}t\right)^{\alpha}$$

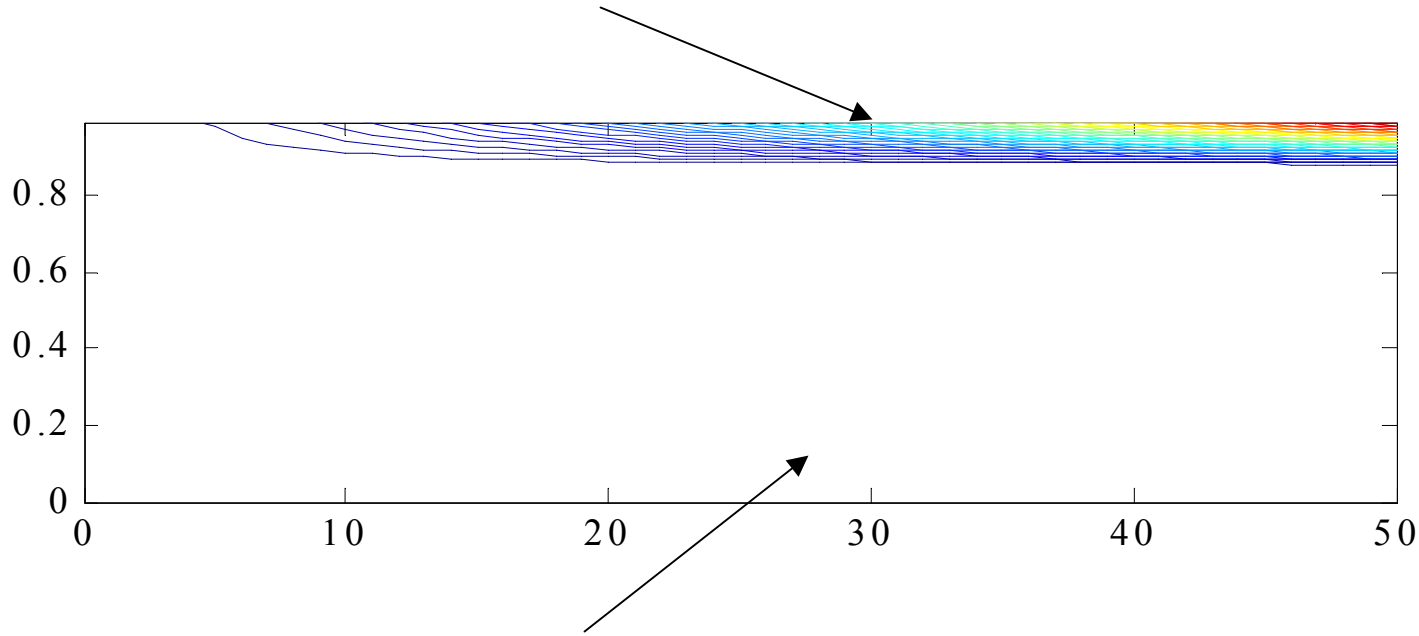
$$R_{\perp} = R_{\perp 0}\left(\dot{\gamma}t\right)^{\beta}$$

$$\alpha = 1.65, \beta = 0.33$$



Drop Size Distribution

Boundary: High Domain Growth



Interior: Low Domain Growth

Summary

- **Injection molding model**
  - » **FIDAP customized for polymer blends**
    - *User defined routines for viscosity and drop size*
    - *Predicts drop size distribution in the injected part from shear distribution*
  - » **Robust injection molding predictions, complex geometry, etc.**
  - » **"Back of the envelope" model**
- **Hierarchical Modeling**
  - » **FIDAP: Compute particle flow paths**
  - » **2-phase flow models: Simulate drop evolution on flow path**
  - » **Compute appropriate averages to define distribution in complex flows**